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EXECUTIVE SUMMARY OF THE THESIS

Dynamic Monte-Carlo Simulations on Anisotropic Ising Systems

LAUREA MAGISTRALE IN ENGINEERING PHYSICS - INGEGNERIA FISICA

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Contents

Introduction

The scope of this thesis is to study the properties of anisotropic spin lattices, i.e. lattices where the exchange interaction in the horizontal direction J_x is different from the one in the vertical direction J_y. This executive summary will cover the most important aspects of this work : first, a description of the 18-fold way algorithm (introduced by NOVOTNY [5]) we used, then the study of dynamic phase transitions the system undergoes when a time-varying sinusoidal external field is applied and finally the impact of introducing randomness into the model is investigated to get a closer look to realistic situations, in order to see how the effect of casualty competes with the anisotropy.

1. State of the art

Anisotropic spin lattices and their implementation, in the last 20 years, have been tackled in several scientific papers that investigated various ways to determine critical parameters of such systems. M. GHAEMI, M. GHANNADI and B. MIRZA [1] computed in 2003 the critical temperature of a multi-layer ferromagnet with anisotropic exchange interaction. They defined three coupling variables : the in-plane exchange constants K_x and K_y and the inter-layer coupling constant K_z and used the Transfer Matrix method. To determine the critical temperature, they plotted the reduced internal energy per site as a function of the reduced temperature for different lattice sizes.

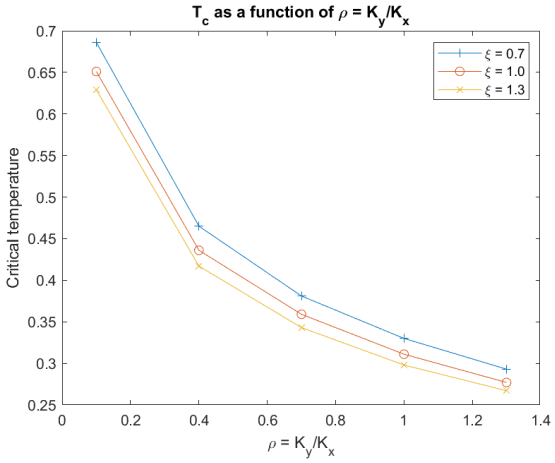

Figure 1: Calculation of the critical temperature by GHAEMI as a function of the anisotropy ([1])

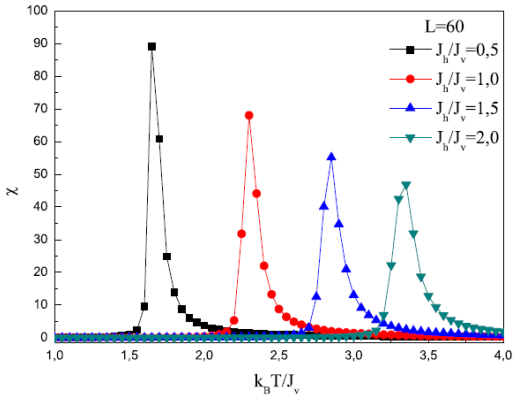

Figure 2: Magnetic susceptibility for different anisotropies (lattice size $L = 60$) ([2])

These curves crossing themselves at the critical point, this allows to recover this parameter.They calculated this parameter for various values of the in-plane anisotropy ratio $\rho = \frac{K_y}{K_x}$ and $\xi = \frac{K_z}{K_x}$. The graph in Fig. 1 shows the computed values within this model for T_c as a function of ρ for different values of the parameter ξ. As we can observe, for a fixed value of ξ, the critical temperature diminishes as the in-plane anisotropy factor ρ increases, in a similar fashion for all three values of ξ. Clearly, the in-plane anisotropy, which is our focus in this thesis (we will simulate 2D lattices) has a higher impact than the inter-layer one : the three curves are pretty close from one another, despite the variation of ξ.
In 2017, D. FARSAL, M. SNINA, M. BADIA and M. BENNAI studied anisotropic spin lattices by the means of two methods : the Finite-Cluster Approximation (FCA) and the Monte-Carlo algorithm. By computing the magnetic susceptibility and finding the position of its peak, they confirmed that the critical temperature undergoes a decreasing trend when the anisotropy goes up, as Fig. 2 shows.

2. 18-fold way algorithm

The classical MONTE-CARLO algorithm for spin lattices is based on single spin-flip, where the spins are all considered as single units. In 1975, LEBOWITZ provided the 10-fold way algorithm, in which the spin lattice is partitioned into 10 classes according to the orientation of the considered spin and to the one of its nearest neighbours. This method allows a better computational efficiency with respect to the classical algorithm. NOVOTNY, in 1995, adapted this partition of a spin lattice to the anisotropic case. In such a configuration, there are exactly 18 classes that form a division of the lattice. If a spin in a given class $i = 1, ..., 18$ is flipped, it will cause a variation of the total energy of the system $\Delta E_i = E_{\text{old}} - E_{\text{new}}$. In order to simulate the dynamic evolution, we use the following probability rates per unit time of spin-flipping for a class i and a spin $s_j = \pm 1$:

$$w_i(s_j) = \frac{1}{2\alpha}\Big(1 + s_j \tanh(\beta \frac{\Delta E_i}{2})\Big), \qquad (1)$$

where $\alpha = 1$ is the inverse of a time (in s^{-1}) and $\beta = \frac{1}{k_B T}$. Such rates correspond to the GLAUBER dynamics : the flips that make the total energy diminish ($\Delta E > 0$) are not accepted with the same probability like with the METROPOLIS dynamics; rather, the ones that correspond to a higher decrease of E are more probable than the others. To check that the algorithm (implemented on MATLAB) works, we need to compare the results we obtain in the static case ($B = 0$) with the analytical prediction made by ONSAGER in 1944:

$$\sinh\Big(\frac{2J_x}{k_B T_c}\Big)\sinh\Big(\frac{2J_y}{k_B T_c}\Big) = 1. \qquad (2)$$

To determine the critical temperature, we calculate the magnetic susceptibility of the system $\chi = \beta(\langle m^2 \rangle - \langle m \rangle^2)$, where $m = \frac{1}{N}\sum_{i,j=1}^{N} s_{i,j}$ is the mean magnetization per spin and $\langle . \rangle$ represents the mean value of a quantity in the canonical ensemble. The curve of χ as a function of

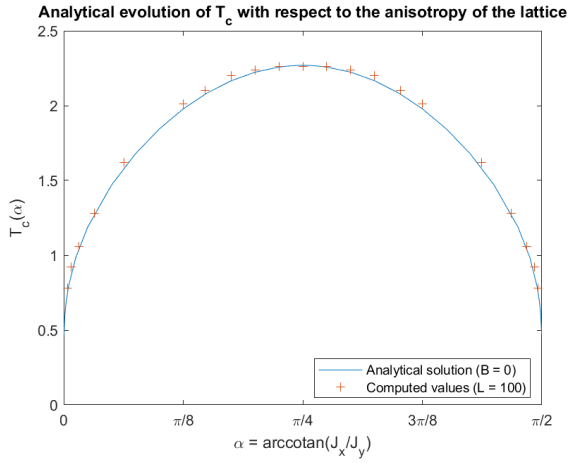

Figure 3: $T_c = f(\alpha)$ (analytical and computed values)

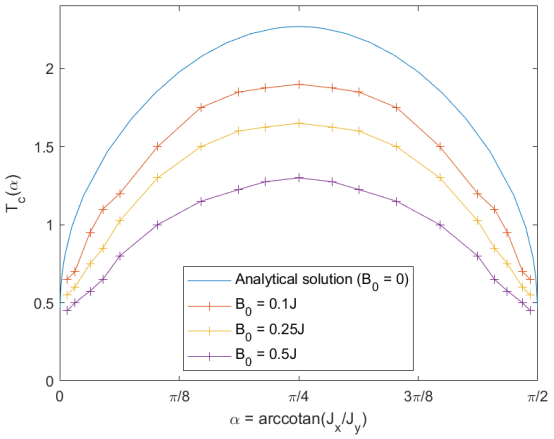

Figure 4: $T_c = f(\alpha)$ (analytical and computed values)

T presenting a peak for $T = T_c$, we can identify the critical temperature for various values of the anisotropy parameter $K = \frac{J_x}{J_y}$. From a physical point of view, having an anisotropy K or $\frac{1}{K}$ should be completely equivalent. Therefore, we impose the following normalization for the two coupling constants

$$\begin{cases} J_x = \sqrt{2}J\cos(\alpha); \\ J_y = \sqrt{2}J\sin(\alpha), \end{cases} \tag{3}$$

where J is taken equal to 1 in our simulation and α (consequently equal to $\text{arccotan}(\frac{J_x}{J_y})$) is the *anisotropy angle*.
Figure 3 shows the values obtained by our simulations with respect to the analytical results predicted by ONSAGER for a lattice of size 100×100, where T_c is plotted as a function of α (the isotropic case being at the center of the graph, for $\alpha = \frac{\pi}{4}$). We observe that our simulations are in line with the theoretical curve, which indicates that the algorithm works well.

3. Dynamic phase transitions

In this section, we analyze the effect of anisotropy on dynamic phase transitions (DPT). DPT occur when a time-varying sinusoidal field $B(t) = B_0\cos(\frac{2\pi}{P}t)$ is applied to the spin lattice. The order parameter in this case is no longer the static magnetization, but the *averaged magnetization per cycle*, also called the dynamic order parameter Q, defined as follows :

$$Q = \frac{1}{P}\oint M(t)dt, \tag{4}$$

where $\oint$ refers to the integral performed over a period of the magnetic field P. The phase transition is occurring at the so-called *dynamic critical temperature* $T_{c,d}$. To determine it, we compute the variance of Q given by

$$\mathcal{V}(Q) = L^2(\langle Q^2\rangle - \langle Q\rangle^2), \tag{5}$$

where L is the length of the square lattice. Similarly to the magnetic susceptibility, this quantity shows a peak for $T = T_{c,d}$. Let us investigate the effect of the field's amplitude and period on the curve $T_c = f(\alpha)$.

3.1. Increasing the field B_0

By fixing the period of the field $P = 1000$ (higher than the spontaneous time constant of the system), we plotted the curves $T_c = f(\alpha)$ for several values of the field's amplitude B_0, as shown on Fig. 4.
As we can see, increasing the field makes the dynamic critical temperature diminish. This is expected, since having a stronger field means bringing a stronger disorder into the system. The effect is very well marked for small anisotropies but is less present on the sides of the diagram. We would have also expected these points to get closer to zero, since $\alpha = 0$ corresponds to a null critical temperature. Since the curves seem to look like the static curve multiplied by a multiplicative factor, we determined for several values of B_0 comprised between 0 and 0.5 the best-fitting factor $a(B_0)$.

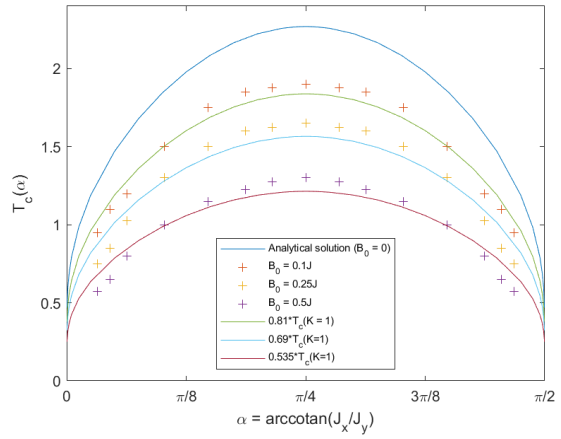

Figure 5: $T_{c,d} = f(\alpha)$ and the best fits $a(B_0) * T_c(B = 0)$

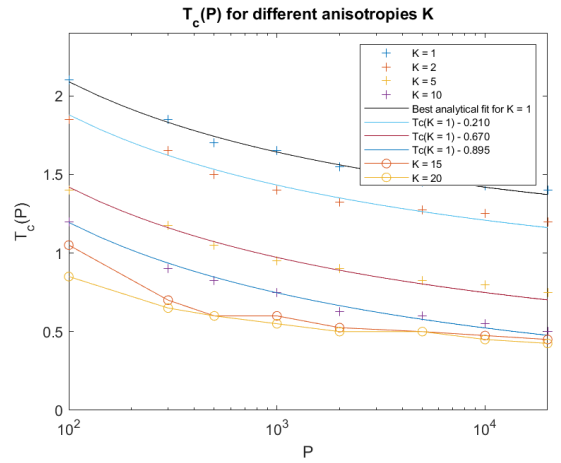

Figure 6: $T_{c,d} = f(P)$ for various anisotropies and the best corresponding fits

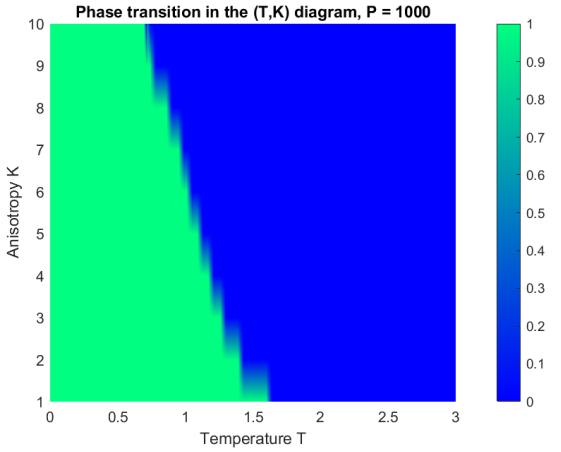

Figure 7: (T, K, Q) 3D phase diagram for $B_0 = 0.3$ and $P = 1000$

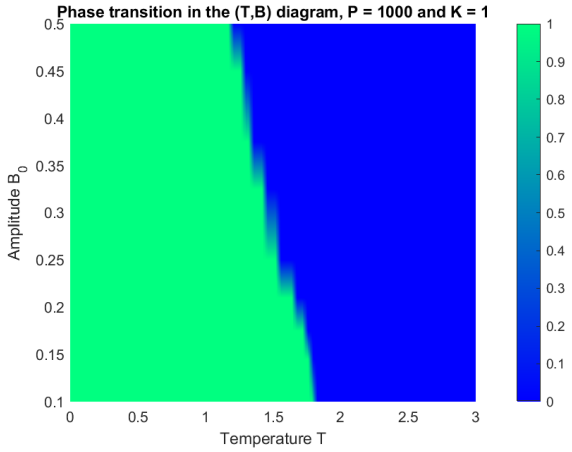

Figure 8: (T, B_0, Q) 3D phase diagram for $K = 1$ and $P = 1000$

Fig. 5 shows the numerical values and the fitting curves for some values of B_0. We observe a fair linear correlation between the coefficients $a(B_0)$ and the values B_0 until $B_0 = 0.5$.

3.2. Decreasing the period P

Another way to make $T_{c,d}$ vary is to decrease the period of the magnetic field. Fixing the amplitude of the magnetic field $B_0 = 0.3$, we determined the dynamic critical temperature for different values of the period (distributed over 2 orders of magnitude to get significant results). Again using the peak of the variance, we obtain the graph shown in Fig. 6.
This graph shows the dynamic critical temperature as a function of the period for various values of the anisotropy factor K. We can extrapolate pretty the points for $K = 1$ with the function $T_c = \frac{a}{\log_{10}(P)} + b$, shown by the black solid line in Fig. 4. The curves $T_{c,d} = f(P)$ show a very similar behaviour, with a constant slope a : they are obtained by a vertical translation of the curve for $K = 1$. This does not seem to hold for stronger anisotropies, as the curves for $K = 15$ and $K = 20$ show a different behaviour for example.

3.3. Phase diagrams

With all the measurements realized in the previous subsections, we were able to draw several phase diagrams between the dynamic ordered phase ($Q = 1$) and the dynamic disordered phase ($Q = 0$) for different configurations : the (T, K, Q) diagram for various values of the field's period, as illustrated by Fig. 7 and the (T, B_0, Q) for various values of the anisotropy factor, on Fig. 8.

4. Random Anisotropy Ising Model

In order to simulate the lattices in a more realistic way, we need to introduce casuality in the model. Indeed, in a real system, the value of the exchange interaction is not uniform across the lattice : it might assume various local values. In analogy with the Random-Bond Ising Model for anisotropic lattices, we introduce an anisotropy carried by the anisotropy angle α, distributed according to a gaussian distribution for a given set of coordinates in the lattice (k,l) :

$$g(\alpha_{k,l}) = \frac{1}{\sqrt{2\pi\sigma_\alpha^2}} e^{-\frac{(\alpha_{k,l}-\bar{\alpha})^2}{2\sigma_\alpha^2}}, \qquad (6)$$

where $\bar{\alpha}$ is the mean of the gaussian distribution, σ_α the standard deviation and R the disorder parameter, on which σ_α depends. To choose a suited value for the standard deviation, we should have a probability of getting a negative angle equal for all mean values $\bar{\alpha}$. By performing analytical calculations, we find that the condition of normalization is to have the standard deviation proportional to the mean value. The associated proportionality coefficient that modulates the randomness is denoted $\sqrt{R}$, where R is called the disorder parameter. The probability of having a negative angle can be plotted and compared with the ferromagnetic limit given in an article by JAGGI as 10 %. Indeed, if there are too much antiferromagnetic links in the lattice ($J < 0$, i.e. $\alpha = 0$), the properties of the lattice become different and the computations we perform would not be applicable anymore. Fig. 9 is showing the probability alongside the ferromagnetic limit, showing that $R^* = 0.6$ constitutes the limit not to overcome in order to stay within the framework of a ferromagnetic lattice.

By considering values of R lower than 0.6, we can find the critical temperature by looking at the position of the magnetic susceptibility's peak. Fig. 10 shows the results of such simulations for $R = 0.1$, 0.2, 0.3 and 0.5. To reduce the bias caused by the fluctuations, we ran ten times each single configuration and plotted the average and the standard deviation of these 10 computations.

The first observation that can be made is that the maximum critical temperature is not in the

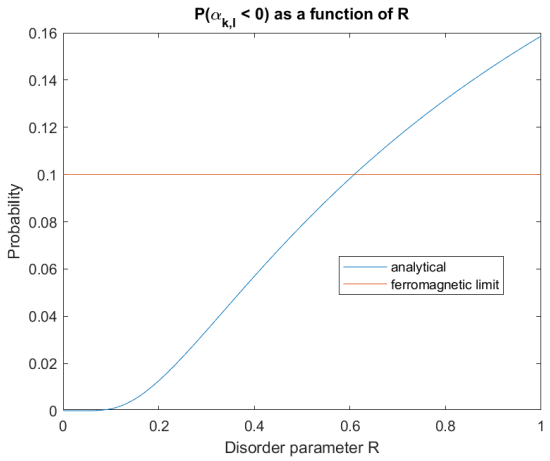

Figure 9: $P(\alpha_{k,l} < 0)$ and the ferromagnetic limit as a function of R

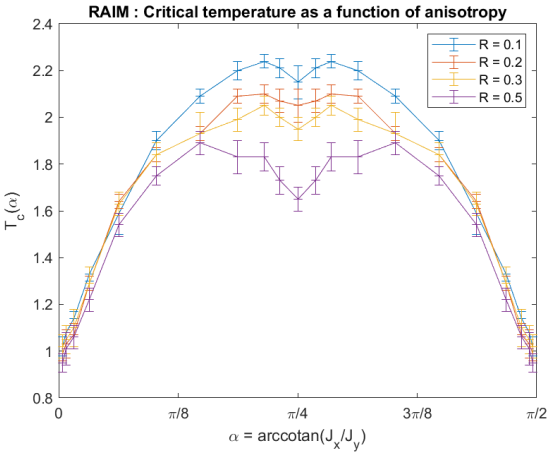

Figure 10: $T_c = f(\bar{\alpha})$ for various values of the disorder parameter

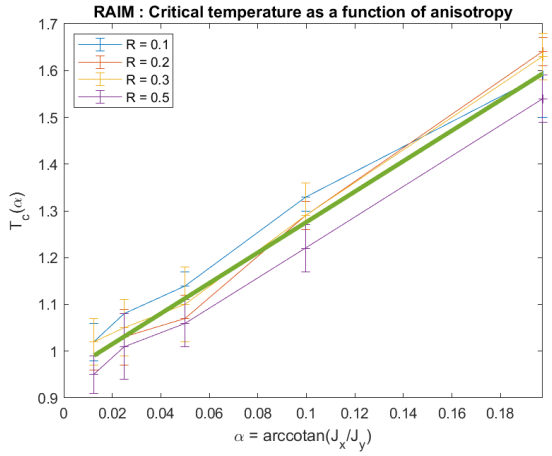

Figure 11: Linear trend for very high anisotropies

center (i.e. the anisotropic case) anymore for a fixed value of R. It gets shifted towards higher mean anisotropies as the disorder parameter increases. Then, we see that the effect of the randomness is limited : when the anisotropy becomes important (typically above $\bar{K} = 10$), the four curves become almost superimposed, with a fair linear trend in this restricted area, as Fig. 11 shows.

Conclusion and future perspectives

To wrap up, the original results of this thesis are multiple :

- the impact of a time-varying sinusoidal magnetic field (its amplitude and its period) on an anisotropic spin lattice;
- the elaboration of multiple three-dimensional phase diagrams for the dynamic order parameter as a function of diverse quantities (the anisotropy factor K, the period P and the amplitude B_0);
- the introduction of the Random-Anisotropy Ising Model to study the impact of randomness in an anisotropic spin lattice.

From the computational point of view, a future perspective would be to write the dynamic algorithm in a parallel way instead of the classical sequential method. Indeed, this would allow to treat way bigger lattices while keeping a small computation time. The idea is to divide the lattice into several regions that are treated by the various processors of the computer that is used for the simulation.

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